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Lobatto IIIA–IIIB discretization of the strongly coupled nonlinear Schrödinger equation

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ABSTRACT

In this paper, we construct a second order semi-explicit multi-symplectic integrator for the strongly coupled nonlinear Schrödinger equation based on the two-stage Lobatto IIIA–IIIB partitioned Runge–Kutta method. Numerical results for different solitary wave solutions including elastic and inelastic collisions, fusion of two solitons and with periodic solutions confirm the excellent long time behavior of the multi-symplectic integrator by preserving global energy, momentum and mass.

1. Introduction

We consider the strongly coupled nonlinear Schrödinger (SCNLS) equation [1–4]

$$\begin{aligned} &\mathrm{i}u_t + \beta u_{xx} + [\alpha_1|u|^2 + (\alpha_1 + 2\alpha_2)|v|^2]u + \gamma u + \Gamma v = 0, \\ &\mathrm{i}v_t + \beta v_{xx} + [\alpha_1|v|^2 + (\alpha_1 + 2\alpha_2)|u|^2]v + \gamma v + \Gamma u = 0, \end{aligned} \tag{1}$$

with the initial conditions

$$u(x, 0) = u_0(x), \qquad v(x, 0) = v_0(x)$$

and the periodic boundary conditions

$$u(x_l, t) = u(x_r, t), \qquad v(x_l, t) = v(x_r, t), \quad t > 0,$$

where $u(x, t)$ and $v(x, t)$ are complex-valued functions of the spatial coordinate x and time t; $\beta, \alpha_1, \alpha_2, \gamma$, and Γ are real constants.

Eq. (1) arises as a system of partial differential equations (pde's) in many problems of mathematical physics, nonlinear optics, solid and fluid mechanics, as well as biological structures. The parameter β describes the group velocity dispersion and the term proportional to α_1 describes the self-focusing of a signal for pulses in birefringent media. The nonlinear coupling or cross-modulation parameter $\alpha = \alpha_1 + 2\alpha_2$ describes how each component of the solution is influenced by the other component. The constant γ is the ambient potential, called normalized birefringent. Finally, the parameter Γ is the linear

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coupling parameter, also called the linear birefringent. The coupling through the terms proportional to Γ is called "strong coupling", which arises in addition to the "weak coupling" through the nonlinear terms [1].

Introduction of the two new parameters γ and Γ enriches the phenomenology of the system. We consider, as in [1] only real values of Γ. This describes additional dispersion due to the coupling in nonlinear optics. Eq. (1) possesses for $\alpha_1 > 0$ multiple sech-like (bright) solutions or for $\alpha_1 < 0$, multiple tanh-like (dark) solutions. We consider only the bright solutions as this was done mostly in the literature. Eq. (1) without the coupling parameter $\Gamma = 0$ is called the Gross–Pitaevskii equation. It was shown that the SCNLS equation (1) is completely integrable for the Manakov case with $\alpha_2 = 0$. Also analytic solutions exits via inverse scattering transformation for the focusing case with $\gamma = \Gamma = \alpha_2 = 0$ [1]. However the non-integrable case with $\alpha_2 \neq 0$ is of importance for understanding the properties of interacting collisions, for example elastic and inelastic soliton collisions.

The SCNLS equation (1) has two standard conserved quantities, namely mass and energy [1,3]. The mass conservation law is obtained by multiplying the first and second equations of (1) by $\overline{u}$ and $\overline{v}$, respectively, collecting the imaginary terms, and then integrating over space. Here $\bar{u}$ and $\bar{v}$ denote the complex conjugates of u and v respectively. This yields

$$\frac{\partial}{\partial t}M(t) = \frac{\partial}{\partial t}\int_{x_l}^{x_r} (|u|^2 + |v|^2)\,\mathrm{d}x = 0. \tag{2}$$

When the coupling parameter $\Gamma \neq 0$ the "masses" of the functions u and v are not conserved separately. Conservation of energy can be obtained by multiplying the first and second equations of (1) by $\overline{u_t}$ and $\overline{v_t}$, respectively, and collecting the real terms, then integrating over space. This yields

$$\begin{aligned}\frac{\partial}{\partial t}E(t) &= \frac{\partial}{\partial t}\frac{1}{2}\int_{x_l}^{x_r}\left[-\beta(|u_x|^2 + |v_x|^2) + \frac{\alpha_1}{2}(|u|^4 + |v|^4) + (\alpha_1 + 2\alpha_2)|u|^2|v|^2 + \gamma(|u|^2 + |v|^2) + 2\Gamma \cdot Re\{\overline{u}v\}\right]\mathrm{d}x \\ &= 0. \end{aligned} \tag{3}$$

As in the case of mass conservation, the energy $E(t)$ is not conserved individually for u and v.

The SCNLS equation was also studied numerically in recent years by applying different conservative schemes. The effect of various parameters on the soliton behavior has been studied numerically. Sonnier and Christov [1] have applied the conservative implicit Crank–Nicholson method (discrete conservation of mass and energy) and obtained for various non-zero parameter values numerical solutions with elastic and non-elastic soliton collisions by setting $\gamma = 0$ and $\alpha_2 = 0$. The same method is used in [2] in complex arithmetic which reduces the computation, and the effect of various parameters was shown numerically. Both methods are second order convergent in space and time variables and require due to implicitness of the schemes, the solution of a system of nonlinear equations at each time step within a given tolerance. Todorrov and Christov [2] investigates numerically the role of linear and nonlinear coupling by taking $\Gamma = 0$. In [3] a second order linearly uncoupled conservative finite difference scheme was used which avoids the solution of nonlinear equations. The mass and energy conservation properties of the scheme are proved in discrete form, and several numerical results are shown for the case with homogeneous Dirichlet boundary conditions by setting $\gamma = 0$. Recently in [4] the implicit Preismannn scheme is developed using the multi-symplectic formulation of the strongly coupled NLS Eq. (1). It is proven that this second order multi-symplectic scheme preserves mass exactly and energy approximately. In this paper we consider non-zero values for all parameters in order to investigate their effect of various soliton behaviors.

Recently, several conservative, symplectic and multi-symplectic integrators were devised for the coupled nonlinear Schrödinger equation (CNLSE) with $\gamma = \Gamma = 0$ [5–12]. The Runge–Kutta (RK) methods play an important role in the numerical solution of symplectic and multi-symplectic pde's. It is shown in [13] that the scalar wave equation can be integrated using concatenation of Gauss–Legendre Runge–Kutta methods in space and time, which leads to a multi-symplectic integrator. It is known that the Preissmann scheme corresponds to the concatenation of the mid-point method in time and space. Similarly the Euler box scheme consists of the symplectic Euler method in space and time. The main weakness of RK based multi-symplectic integrators is that their implicit nature causes theoretical and practical problems due to the solutions of large nonlinear systems [14,15]. Another useful class of multi-symplectic integrators is the partitioned Runge–Kutta (PRK) methods which are applied successfully to symplectic ordinary differential equations (ode's) which may yield explicit methods for some nonlinear pde's. It is shown in [14,15] that the partitioned Lobatto IIIA–IIIB methods yield well defined multi-symplectic integrators for some nonlinear Hamiltonian equations like the the NLS, Bossinesque [16] and KdV equations. Here we apply the two-stage second order Lobatto IIIA–IIIB method to the SCLNS equation using a different partitioning of the variables in space and time discretization. The resulting scheme is a semi-explicit multi-symplectic integrator, requiring only one Newton iteration at each time step, which is more efficient than a fully implicit conservative and multi-symplectic scheme such as the Preissmann scheme.

The paper is organized as follows. In Section 2 we give the multi-symplectic formulation of the SCNLS equation. The two stage Lobatto IIIA–IIIB method as a multi-symplectic integrator is then applied to the SCNLS equation. The fully discretized equations in space and time are given with the discrete multi-symplectic conservation law in Section 2. In Section 3 we present numerical results for elastic and inelastic soliton collisions, fusion of solitons and for periodic solutions by using various parameters. The paper ends with some conclusions in Section 4.

2. Multi-symplectic formulation of SCNLS equation and multi-symplectic integration

2.1. Multi-symplectic formulation of the SCNLS equation

By decomposing the complex functions u and v into real and imaginary parts

$$u = p + \mathrm{i}q, \quad v = \mu + \mathrm{i}\xi$$

the SCNLS equation (1) can be written as a system of real-valued equations

$$\begin{aligned}
&-q_t + \beta\, p_{xx} + (\alpha_1(p^2+q^2) + \alpha(\mu^2+\xi^2))p + \gamma p + \Gamma\mu = 0,\\
&p_t + \beta\, q_{xx} + (\alpha_1(p^2+q^2) + \alpha(\mu^2+\xi^2))q + \gamma q + \Gamma\xi = 0,\\
&-\xi_t + \beta\, \mu_{xx} + (\alpha_1(\mu^2+\xi^2) + \alpha(p^2+q^2))\mu + \gamma\mu + \Gamma p = 0,\\
&\mu_t + \beta\, \xi_{xx} + (\alpha_1(\mu^2+\xi^2) + \alpha(p^2+q^2))\xi + \gamma\xi + \Gamma q = 0.
\end{aligned} \tag{4}$$

After introducing new variables $\beta\, u_x = b + \mathrm{i}\, a$, $\beta\, v_x = d + \mathrm{i}\, c$ the multi-symplectic formulation can be given as

$$\mathbf{K} z_t + \mathbf{L} z_x = \nabla_{\mathbf{z}} S(\mathbf{z}) \tag{5}$$

with the state variables $\mathbf{z} = (p, \mu, q, \xi, b, d, a, c)^T$ and the skew-symmetric matrices

$$\mathbf{K} = \begin{pmatrix} \mathbf{0} & -\mathbf{I_2} & \mathbf{0} & \mathbf{0} \\ \mathbf{I_2} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \qquad \mathbf{L} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{I_2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I_2} \\ -\mathbf{I_2} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I_2} & \mathbf{0} & \mathbf{0} \end{pmatrix} \tag{6}$$

where $\mathbf{0}$, $\mathbf{I_2}$ are 2×2 zero and identity matrices respectively. The Hamiltonian function $S(z) : R^8 \to R$, is given by

$$\begin{aligned}
S(\mathbf{z}) = &-\frac{\alpha_1}{4}(p^2+q^2)^2 - \frac{\alpha_1}{4}(\mu^2+\xi^2)^2 - \left(\frac{\alpha_1 + 2\alpha_2}{2}\right)(p^2+q^2)(\mu^2+\xi^2)\\
&- \frac{\gamma}{2}(p^2+q^2+\mu^2+\xi^2) - \Gamma(p\mu + q\xi) - \frac{1}{2\beta}(a^2+b^2+c^2+d^2).
\end{aligned} \tag{7}$$

The SCNLS equation in multi-symplectic form (5) satisfies the multi-symplectic conservation law

$$\omega_t + \kappa_x = 0 \quad \text{with } \omega = \frac{1}{2}\mathrm{d}\mathbf{z} \wedge \mathbf{K}\mathrm{d}\mathbf{z} \quad \text{and} \quad \kappa = \frac{1}{2}\mathrm{d}\mathbf{z} \wedge \mathbf{L}\mathrm{d}\mathbf{z} \tag{8}$$

together with a local energy and local momentum conservation laws

$$\begin{aligned}
&E_t + F_x = 0, \qquad E(\mathbf{z}) = S(\mathbf{z}) + \frac{1}{2}\mathbf{z}_x^T \mathbf{L}\mathbf{z}, \qquad F(\mathbf{z}) = -\frac{1}{2}\mathbf{z}_t \mathbf{L}\mathbf{z},\\
&I_t + G_x = 0, \qquad G(\mathbf{z}) = S(\mathbf{z}) + \frac{1}{2}\mathbf{z}_t^T \mathbf{K}\mathbf{z}, \qquad I(\mathbf{z}) = -\frac{1}{2}\mathbf{z}_x \mathbf{K}\mathbf{z},
\end{aligned} \tag{9}$$

$$E(\mathbf{z}) = S(\mathbf{z}) + \frac{1}{\beta}(a^2+b^2+c^2+d^2), \qquad F(\mathbf{z}) = -bp_t - d\mu_t - aq_t - c\xi_t$$

$$I(\mathbf{z}) = \frac{1}{2\beta}(qb + \xi d - pa - \mu c), \qquad G(\mathbf{z}) = S(\mathbf{z}) - \frac{1}{2}(qp_t + \xi\mu_t - pq_t - \mu\xi_t).$$

It has been shown that discretizing the multi-symplectic pde (5) in space and time with partitioned Runge–Kutta methods gives rise to a system of equations that formally satisfy a discrete multi-symplectic conservation law. This kind of discretization uses the same partitioning of the variables in both space and time discretization, and in general is fully implicit. In [15], Ryland and McLachlan give sufficient conditions on a multi-symplectic pde for a Lobatto IIIA–IIIB discretization in space to give rise to explicit ode's, and an algorithm for constructing these ode's. In this discretization the variables are partitioned independently in space and time.

Theorem 2.1 ([15])**.** *Consider a multi-symplectic pde* (5)*, where the matrices* $\mathbf{K}$ *and* $\mathbf{L}$ *have the following structures:*

$$\mathbf{K} = \begin{pmatrix} & -\mathbf{I}_{\frac{1}{2}(d_1+d_2)} & \\ \mathbf{I}_{\frac{1}{2}(d_1+d_2)} & & \\ & & \mathbf{0}_{d_1} \end{pmatrix}, \qquad \mathbf{L} = \begin{pmatrix} & & \mathbf{I}_{d_1} \\ & \mathbf{0}_{d_2} & \\ -\mathbf{I}_{d_1} & & \end{pmatrix} \tag{10}$$

where $d_1 = n - \mathrm{rank}(\mathbf{K})$, $d_2 = n - 2d_1 \le d_1$, $\mathbf{I}_d$ *and* $\mathbf{0}_d$ *are the* $d \times d$ *identity and zero matrices respectively.*

Let the variable $\mathbf{z}$ *be partitioned into two parts* $\mathbf{z}^{(1)} \in \mathbb{R}^{d_1+d_2}$ *and* $\mathbf{z}^{(2)} \in \mathbb{R}^{d_1}$*, where we denote the first* d_1 *component of* $\mathbf{z}^{(1)}$ *by* $\mathbf{q}$*, the last* d_2 *components of* $\mathbf{z}^{(1)}$ *by* $\mathbf{v}$*, and the components of* $\mathbf{z}^{(2)}$ *by* $\mathbf{p}$ *such that the PDE may be written as*

$$\begin{pmatrix} & -\mathbf{I}_{\frac{1}{2}(d_1+d_2)} & \\ \mathbf{I}_{\frac{1}{2}(d_1+d_2)} & & \\ & & \mathbf{0}_{d_1} \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{v} \\ \mathbf{p} \end{pmatrix}_t + \begin{pmatrix} & & \mathbf{I}_{d_1} \\ & \mathbf{0}_{d_2} & \\ -\mathbf{I}_{d_1} & & \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{v} \\ \mathbf{p} \end{pmatrix}_x = \begin{pmatrix} \nabla_{\mathbf{q}} S(\mathbf{z}) \\ \nabla_{\mathbf{v}} S(\mathbf{z}) \\ \nabla_{\mathbf{p}} S(\mathbf{z}) \end{pmatrix}. \tag{11}$$

If the function $S(\mathbf{z})$ *can be written in the form*

$$S(\mathbf{z}) = T(\mathbf{p}) + V(\mathbf{q}) + \widehat{V}(\bar{\mathbf{v}}) \tag{12}$$

where $T(\mathbf{p}) = \frac{1}{2}\mathbf{p}^T \Lambda \mathbf{p}$ *and* $\widehat{V}(\mathbf{v}) = \frac{1}{2}\mathbf{v}^T \alpha \mathbf{v}$ *such that* $|\Lambda| \neq 0$ *and* $|\alpha| \neq 0$*, then applying an* r*-stage Lobatto* IIIA–IIIB *PRK discretization in space to the pde leads to a set of explicit local ode's in time in the stage variables associated with* $\mathbf{q}$.

Comparing the matrices $\mathbf{K}$ and $\mathbf{L}$ in (6) of the SCNLS equation (5) with (10) we see that $d_1 = 4$ and $d_2 = 0$ with $\mathbf{z}^{(1)} = \mathbf{q} = \{p, \mu, q, \xi\}$ and $\mathbf{z}^{(2)} = \mathbf{p} = \{b, d, a, c\}$. $S(\mathbf{z})$ can be written as (12) with

$$V(\mathbf{q}) = -\frac{\alpha_1}{4}(p^2+q^2)^2 - \frac{\alpha_1}{4}(\mu^2+\xi^2)^2 - \left(\frac{\alpha^2}{2}\right)(p^2+q^2)(\mu^2+\xi^2) - \frac{\gamma}{2}(p^2+q^2+\mu^2+\xi^2) - \Gamma(p\mu+q\xi)$$

and $T(\mathbf{p}) = \frac{1}{2}\mathbf{p}^T\,\Lambda\,\mathbf{p}$ where

$$\Lambda = \begin{pmatrix} -1/\beta & 0 & 0 & 0 \\ 0 & -1/\beta & 0 & 0 \\ 0 & 0 & -1/\beta & 0 \\ 0 & 0 & 0 & -1/\beta \end{pmatrix} \quad \text{and} \quad \mathbf{p} = \begin{pmatrix} b \\ d \\ a \\ c \end{pmatrix}.$$

Because $d_2 = 0$, there are no terms with $\hat{v}$. Thus the SCNLS equation satisfies the requirements of the Theorem 2.1. The system (5) of pde's is then discretized in the spatial variable by the 2-stage Lobatto IIIA–IIIB PRK method, which corresponds to the table

$$\text{IIIA:}\ \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}\,, \qquad \text{IIIB:}\ \begin{array}{c|cc} 0 & 1/2 & 0 \\ 1 & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array}\,. \tag{13}$$

After elimination of the stage variables associated with $\mathbf{p} = \{b, d, a, c\}$ and rearranging the resulting equations, we obtain the explicit local ode's in time for the stage variables associated with $\mathbf{q} = \{p, \mu, q, \xi\}$, namely

$$\begin{aligned}
\partial_t q_i &= \beta\frac{p_{i-1} - 2p_i + p_{i+1}}{\Delta x^2} + (\alpha_1(p_i^2+q_i^2) + \alpha(\mu_i^2+\xi_i^2))p_i + \gamma p_i + \Gamma\mu_i, \\
\partial_t p_i &= -\beta\frac{q_{i-1} - 2q_i + q_{i+1}}{\Delta x^2} - (\alpha_1(p_i^2+q_i^2) + \alpha(\mu_i^2+\xi_i^2))q_i - \gamma q_i - \Gamma\xi_i, \\
\partial_t \xi_i &= \beta\frac{\mu_{i-1} - 2\mu_i + \mu_{i+1}}{\Delta x^2} + (\alpha_1(\mu_i^2+\xi_i^2) + \alpha(p_i^2+q_i^2))\mu_i + \gamma\mu_i + \Gamma p_i \\
\partial_t \mu_i &= -\beta\frac{\xi_{i-1} - 2\xi_i + \xi_{i+1}}{\Delta x^2} - (\alpha_1(\mu_i^2+\xi_i^2) + \alpha(p_i^2+q_i^2))\xi_i - \gamma\xi_i - \Gamma q_i.
\end{aligned} \tag{14}$$

We note that Lobatto IIIA–IIIB semi-discretization in time corresponds to replacing the p_{xx}, q_{xx}, μ_{xx} and ξ_{xx} terms in Eq. (4) by the central difference discretization.

The ode's (14) satisfy the semi-discrete multi-symplectic conservation law

$$\begin{aligned}
&\partial_t(dp_i \wedge dq_i + d\mu_i \wedge d\xi_i) + \frac{\beta}{\Delta x^2}[(dq_{i+1} + dq_{i-1}) \wedge dq_i + (dp_{i+1} + dp_{i-1}) \wedge dp_i \\
&\quad + (d\xi_{i+1} + d\xi_{i-1}) \wedge d\xi_i + (d\mu_{i+1} + d\mu_{i-1}) \wedge d\mu_i] = 0.
\end{aligned} \tag{15}$$

This is a direct consequence of Eq. (14) as it was shown for the uncoupled NLS equation in [17].

We will now consider the time integration of the ode's (14) by the second order Lobatto IIIA–IIIB methods (13). For a system of ode's

$$\mathbf{r}_t = f(\mathbf{r}, \mathbf{s}), \qquad \mathbf{s}_t = g(\mathbf{r}, \mathbf{s})$$

applying Lobatto IIIA to the variable $\mathbf{r}$ and Lobatto IIIB to the variable $\mathbf{s}$ is known as the generalized leapfrog method [15]:

$$\begin{aligned}
\mathbf{r}^{n+\frac{1}{2}} &= \mathbf{r}^n + \frac{\Delta t}{2} f(\mathbf{r}^{n+\frac{1}{2}}, \mathbf{s}^n), \\
\mathbf{s}^{n+1} &= \mathbf{s}^n + \frac{\Delta t}{2}(g(\mathbf{r}^{n+\frac{1}{2}}, \mathbf{s}^n) + g(\mathbf{r}^{n+\frac{1}{2}}, \mathbf{s}^{n+1})), \\
\mathbf{r}^{n+1} &= \mathbf{r}^{n+\frac{1}{2}} + \frac{\Delta t}{2} f(\mathbf{r}^{n+\frac{1}{2}}, \mathbf{s}^{n+1}),
\end{aligned} \tag{16}$$

which is in general an implicit method.

We choose now different partitioning $\mathbf{z}^{(3)} = (p, \mu, b, d)$ and $\mathbf{z}^{(4)} = (q, \xi, a, c)$ for the discretization of the semi-discretized system (14). The variables a, b, c and d have been eliminated in (14). Applying the Lobatto IIIA method to the variables in $\mathbf{z}^{(3)}$ and the Lobatto IIIB method to the variables $\mathbf{z}^{(4)}$ we obtain an integrator which maps $(p_i^n, q_i^n, \xi_i^n, \mu_i^n)$ to $(p_i^{n+1}, q_i^{n+1}, \xi_i^{n+1}, \mu_i^{n+1})$ according to

$$\begin{aligned}
q_i^{n+\frac{1}{2}} &= q_i^n + \frac{\Delta t}{2}\left[\frac{\beta}{\Delta x^2}(p_{i+1}^n - 2p_i^n + p_{i-1}^n) + Z_1 p_i^n + \Gamma \mu_i^n\right] \\
\xi_i^{n+\frac{1}{2}} &= \xi_i^n + \frac{\Delta t}{2}\left[\frac{\beta}{\Delta x^2}(\mu_{i+1}^n - 2\mu_i^n + \mu_{i-1}^n) + Z_2 \mu_i^n + \Gamma p_i^n\right] \\
p_i^{n+1} &= p_i^n - \frac{\Delta t}{2}\left[\frac{2\beta}{\Delta x^2}(q_{i+1}^{n+\frac{1}{2}} - 2q_i^{n+\frac{1}{2}} + q_{i-1}^{n+\frac{1}{2}}) + Z_3 q_i^{n+\frac{1}{2}} + 2\Gamma \xi_i^{n+\frac{1}{2}}\right] \\
\mu_i^{n+1} &= \mu_i^n - \frac{\Delta t}{2}\left[\frac{2\beta}{\Delta x^2}(\xi_{i+1}^{n+\frac{1}{2}} - 2\xi_i^{n+\frac{1}{2}} + \xi_{i-1}^{n+\frac{1}{2}}) + Z_4 \xi_i^{n+\frac{1}{2}} + 2\Gamma q_i^{n+\frac{1}{2}}\right] \\
q_i^{n+1} &= q_i^{n+\frac{1}{2}} + \frac{\Delta t}{2}\left[\frac{\beta}{\Delta x^2}(p_{i+1}^{n+1} - 2p_i^{n+1} + p_{i-1}^{n+1}) + Z_5 p_i^{n+1} + \Gamma \mu_i^{n+1}\right] \\
\xi_i^{n+1} &= \xi_i^{n+\frac{1}{2}} + \frac{\Delta t}{2}\left[\frac{\beta}{\Delta x^2}(\mu_{i+1}^{n+1} - 2\mu_i^{n+1} + \mu_{i-1}^{n+1}) + Z_6 \mu_i^{n+1} + \Gamma p_i^{n+1}\right]
\end{aligned} \tag{17}$$

where

$$\begin{aligned}
Z_1 &= \alpha_1((p_i^n)^2 + (q_i^{n+\frac{1}{2}})^2) + (\alpha_1 + 2\alpha_2)\,((\mu_i^n)^2 + (\xi_i^n)^2) + \gamma \\
Z_2 &= \alpha_1((\mu_i^n)^2 + (\xi_i^{n+\frac{1}{2}})^2) + (\alpha_1 + 2\alpha_2)\,((p_i^n)^2 + (q_i^{n+\frac{1}{2}})^2) + \gamma \\
Z_3 &= \alpha_1((p_i^n)^2 + (q_i^{n+\frac{1}{2}})^2) + (\alpha_1 + 2\alpha_2)\,((\mu_i^n)^2 + (\xi_i^{n+\frac{1}{2}})^2) \\
&\quad + \alpha_1((p_i^{n+1})^2 + (q_i^{n+\frac{1}{2}})^2) + (\alpha_1 + 2\alpha_2)\,((\mu_i^n)^2 + (\xi_i^{n+\frac{1}{2}})^2) + 2\gamma \\
Z_4 &= \alpha_1((\mu_i^n)^2 + (\xi_i^{n+\frac{1}{2}})^2) + (\alpha_1 + 2\alpha_2)\,((p_i^{n+1})^2 + (q_i^{n+\frac{1}{2}})^2) \\
&\quad + \alpha_1((\mu_i^{n+1})^2 + (\xi_i^{n+\frac{1}{2}})^2) + (\alpha_1 + 2\alpha_2)\,((p_i^{n+1})^2 + (q_i^{n+\frac{1}{2}})^2) + 2\gamma \\
Z_5 &= \alpha_1((p_i^{n+1})^2 + (q_i^{n+\frac{1}{2}})^2) + (\alpha_1 + 2\alpha_2)\,((\mu_i^{n+1})^2 + (\xi_i^{n+\frac{1}{2}})^2) + \gamma \\
Z_6 &= \alpha_1((\mu_i^{n+1})^2 + (\xi_i^{n+\frac{1}{2}})^2) + (\alpha_1 + 2\alpha_2)\,((p_i^{n+1})^2 + (q_i^{n+1})^2) + \gamma.
\end{aligned}$$

The variables $\mathbf{r}$, $\mathbf{s}$ in Eq. (16) correspond to $\mathbf{r} = (q, \xi)$ and $\mathbf{s} = (p, \mu)$ in Eq. (17), respectively. Thus, with the above partitioning of the variables, semi-explicit multi-symplectic integrator for SCNLS can be constructed by applying a 2-stage Lobatto IIIA–IIIB discretization in space and generalized leap-frog in time. The resulting scheme is a nine-point, three time level multi-symplectic integrator. In the case of the uncoupled NLS equation, one obtains for a 2-stage Lobatto IIIA–IIIB discretization a pair of quadratic equations, which can be solved explicitly as it was mentioned in [17]. The quadratic equations were solved there by an explicit integrator imposing step size restrictions in the time direction $\Delta t < C(\Delta x)^2$ to preserve the numerical stability. We have used here Newton iteration for solving the quadratic nonlinearities. It was shown in [18] for solving quadratic nonlinearties, resulting by midpoint discretization, theoretically (in exact arithmetic) one Newton iteration would be sufficient. Because of the roundoff errors, here we have applied more than one Newton iteration with the tolerance $tol = 10^{-5}$ as stopping criteria, to solve the quadratic nonlinearities $q_i^{n+1/2}$, $\xi_i^{n+1/2}$, p_i^{n+1}, μ_i^{n+1} in Eq. (17). In all numerical experiments, at most two or three Newton iterations were required to solve the quadratic nonlinearities in Eq. (17) within the given accuracy. The linear parts in Eq. (17) can be integrated explicitly. Therefore the whole scheme is a semi-explicit one. In contrast to this, the implicit multi-symplectic methods like the Preismann scheme require more Newton steps than the Lobatto IIIA–IIIB discretization in order to find an approximate solution.

For second order Lobatto IIIA–IIIB with partitioning $\{(p, \mu, q, \xi), (b, d, a, c)\}$ in space and $\{(p, \mu, b, d), (q, \xi, a, c)\}$ in time applied to the SCNLS (1) the discrete multi-symplectic conservation law in terms of the local values of p, q, μ and ξ is

$$\begin{aligned}
&\left(\frac{1}{\Delta t} + \alpha_1 p_i^{n+1} q_i^{n+\frac{1}{2}}\right) dp_i^{n+1} \wedge dq_i^{n+\frac{1}{2}} + \left(\frac{1}{\Delta t} + \alpha_1 \mu_i^{n+1} \xi_i^{n+\frac{1}{2}}\right) d\mu_i^{n+1} \wedge d\xi_i^{n+\frac{1}{2}} \\
&- \left(\frac{1}{\Delta t} + \alpha_1 p_i^n q_i^{n-\frac{1}{2}}\right) dp_i^n \wedge dq_i^{n-\frac{1}{2}} - \left(\frac{1}{\Delta t} + \alpha_1 \mu_i^n \xi_i^{n-\frac{1}{2}}\right) d\mu_i^n \wedge d\xi_i^{n-\frac{1}{2}} \\
&+ (\alpha_1 + 2\alpha_2)\,(p_i^{n+1} \xi_i^{n+\frac{1}{2}} dp_i^{n+1} \wedge d\xi_i^{n+\frac{1}{2}} + \mu_i^{n+1} q_i^{n+1} d\mu_i^{n+1} \wedge dq_i^{n+1}) \\
&- (\alpha_1 + 2\alpha_2)\,(p_i^n \xi_i^{n-\frac{1}{2}} dp_i^n \wedge d\xi_i^{n-\frac{1}{2}} + \mu_i^n q_i^n d\mu_i^n \wedge dq_i^n)
\end{aligned}$$

$$+\frac{\beta}{\Delta x^2}((dp_{i+1}^n + dp_{i-1}^n) \wedge dp_i^n + (d\mu_{i+1}^n + d\mu_{i-1}^n) \wedge d\mu_i^n)$$
$$+\frac{\beta}{\Delta x^2}((dq_{i+1}^{n+\frac{1}{2}} + dq_{i-1}^{n+\frac{1}{2}}) \wedge dq_i^{n+\frac{1}{2}} + (d\xi_{i+1}^{n+\frac{1}{2}} + d\xi_{i-1}^{n+\frac{1}{2}}) \wedge d\xi_i^{n+\frac{1}{2}}) = 0. \quad (18)$$

This can be verified directly by substituting Eq. (17) into Eq. (18) as it was done for the uncoupled NLS equation in [17].

3. Numerical results

In order to investigate the performance of the multi-symplectic integrator developed in Section 2, in the numerical calculations we chose non-zero values for the parameter α_2, γ and Γ. In all numerical examples we fixed the $\beta = 1.0$, $\alpha_1 = 1.0$, $\gamma = 1.0$. We have observed elastic collisions for the parameters $\alpha_2 = -1/6$, $\Gamma = 1.0$ and inelastic collisions for $\alpha_2 = -1/6$, $\Gamma = 0.0175$. The choice of the parameters $\alpha_2 = -1/3$, $\Gamma = 0.0175$ resulted in the fusion of two solitons.

The space interval $[x_l, x_r]$ is discretized by $N+1$ uniform grid points with grid spacing $\Delta x = h = (x_r - x_l)/N$. We compute the solution for the time interval $0 \le t \le T$. The accuracy of the scheme is tested by calculating the discrete analogues of the global energy and momentum

$$GE = \Delta x \sum_{i=1}^{N} (E_i^n - E_i^0), \qquad GI = \Delta x \sum_{i=1}^{N} (I_i^n - I_i^0) \quad (19)$$

where E^0 and I^0 are the initial energy and momentum respectively and

$$E_i^n = S(\mathbf{z_i^n}) + \frac{1}{\beta}((a_i^n)^2 + (b_i^n)^2 + (c_i^n)^2 + (d_i^n)^2),$$
$$I_i^n = \frac{1}{2\beta}(q_i^n b_i^n + \xi_i^n d_i^n - p_i^n a_i^n - \mu_i^n c_i^n)$$

are the energy and momentum at $t = n\Delta t$ by the proposed scheme.

Elastic collisions: Elastic collisions are those from which the newly formed shapes reemerge under deformation. First, we consider the elastic collision of two solitons by choosing the parameters $\beta = 1.0$, $\alpha_1 = 1.0$, $\alpha_1 = -1/6$, $\gamma = 1.0$, $\Gamma = 1.0$, and taking as the initial conditions

$$u(0,x) = \sqrt{2}\,\mathrm{sech}\left(x + \frac{1}{2}D_0\right) e^{iV_0 x/4}$$
$$v(0,x) = \sqrt{2}\,\mathrm{sech}\left(x - \frac{1}{2}D_0\right) e^{-iV_0 x/4} \quad (20)$$

with $D_0 = 25$ and $V_0 = 1.0$.

Fig. 1 shows that the proposed scheme simulates the solitary waves well. The two waves emerge without any changes in their shapes. This phenomenon shows that the interaction is elastic. Fig. 2 represents the errors in global energy and momentum conservations. We see that the energy and momentum are well preserved and we have observed fluctuations after collisions. We notice that the collision takes place near $t = 25$ at which the errors are corrupted. Moreover, the error increases when the collision takes place, but the errors in the energy and momentum return to small oscillations near zero.

Inelastic collision: When additional oscillations occur after the collision in the initial wave form, it is referred to as an inelastic collision. Now we consider the inelastic-transitive collision of two solitons. To do so, we choose the parameters $\beta = 1.0$, $\alpha_1 = 1.0$, $\alpha_1 = -1/6$, $\gamma = 1.0$, $\Gamma = 0.0175$ in (1) and consider the same initial condition (20) with $D_0 = 25$, $V_0 = 1.0$.

Fig. 3 shows inelastic collision of two solitons. From this figure we see that, after the interaction, the solitary waves leave dispersive oscillations and their amplitudes are altered. Both waves change their shape and the interaction is inelastic. Fig. 4 represents the global energy and momentum conservation.

Fusion of two solitons: We consider now the fusion of the two solitons by choosing the parameters $\beta = 1.0$, $\alpha_1 = 1.0$, $\alpha_1 = -1/3$, $\gamma = 1.0$, $\Gamma = 0.0175$ in (1) and use the same initial condition (20) with $D_0 = 20$, $V_0 = 0.4$. From Fig. 5 we see that the two solitons collapse into one soliton. Fig. 6 represents the global energy and momentum conservation.

Periodic solutions: Finally, we consider the periodic solution of the SCNLS equation (1) by choosing the parameters as

$$\beta = 1.0, \qquad \alpha_1 = 1.0, \qquad \alpha_1 = -1/6, \qquad \gamma = 1.0, \qquad \Gamma = 0.175$$

and taking as the initial condition

$$u(0,x) = a_0(1 - \epsilon\cos(\ell x)), \qquad v(0,x) = b_0(1 - \epsilon\cos(\ell x)) \quad (21)$$

with $a_0 = 0.5$, $b_0 = 0.5$, $\epsilon = 0.1$ and $\ell = 0.5$.

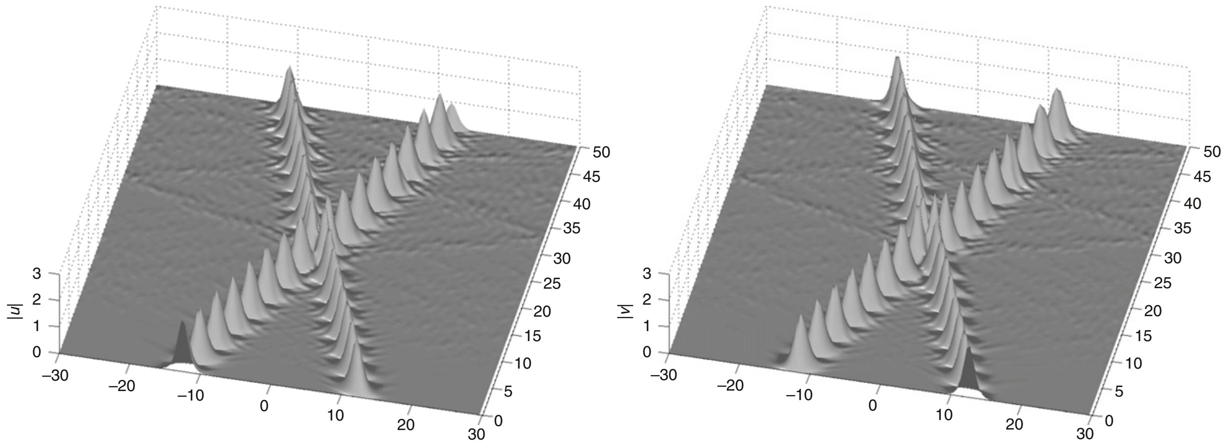

Fig. 1. Elastic collision of two solitons with $\alpha_1 = 1.0, \alpha_2 = -1/6, \gamma = 1.0$ and $\Gamma = 1.0$.

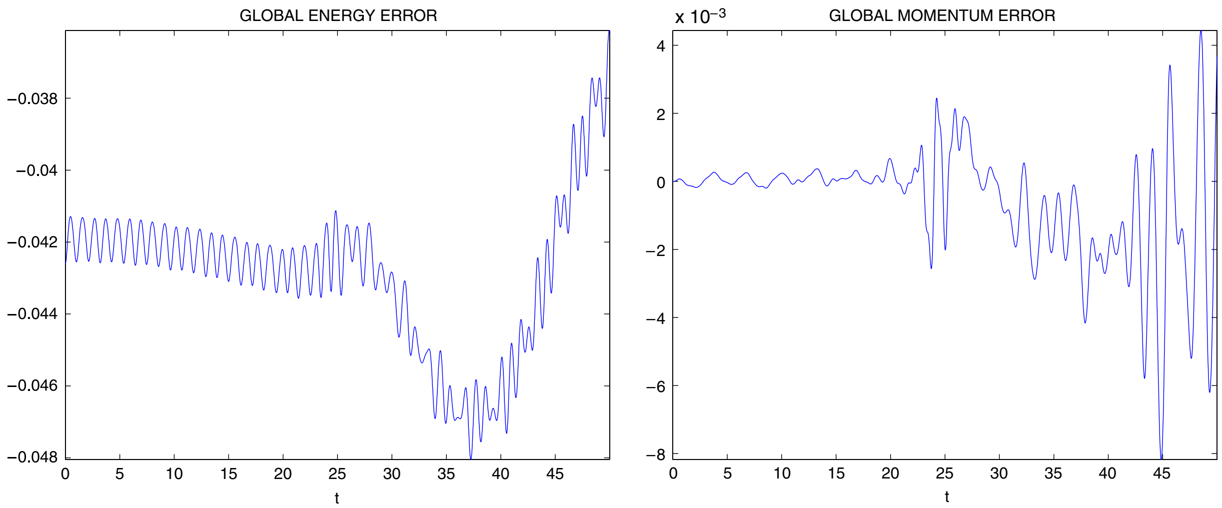

Fig. 2. Global errors for the elastic collision of two solitons.

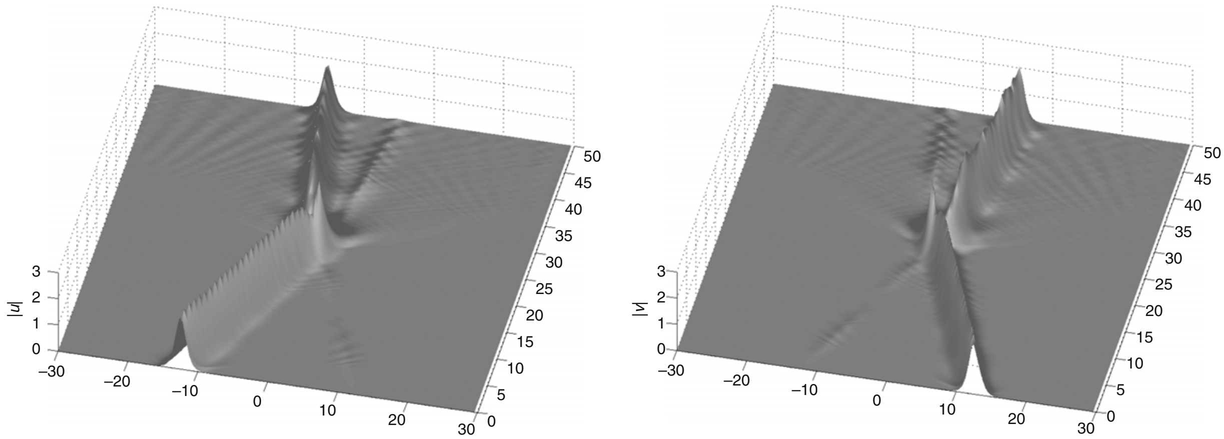

Fig. 3. Inelastic collision of two solitons with $\alpha_1 = 1.0, \alpha_2 = -1/6, \gamma = 1.0$ and $\Gamma = 0.0175$.

Fig. 7 shows quasi-periodic breather motion. Fig. 8 represents the global energy and momentum conservation. From this figure we see that there is no a drift in energy conservation in contrast to the non-conservative integrators. In case of

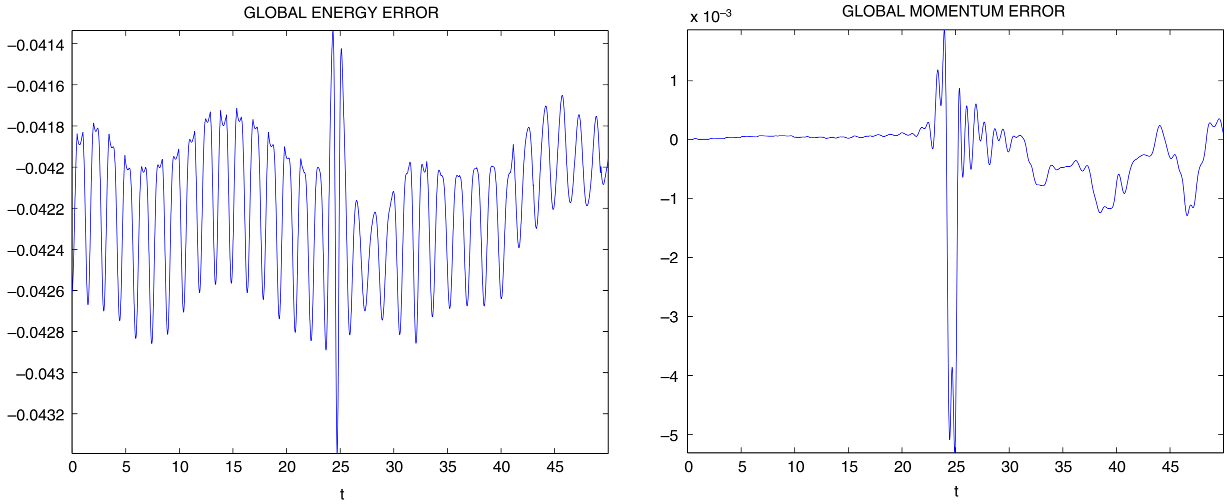

Fig. 4. Global errors for the inelastic collision of two solitons.

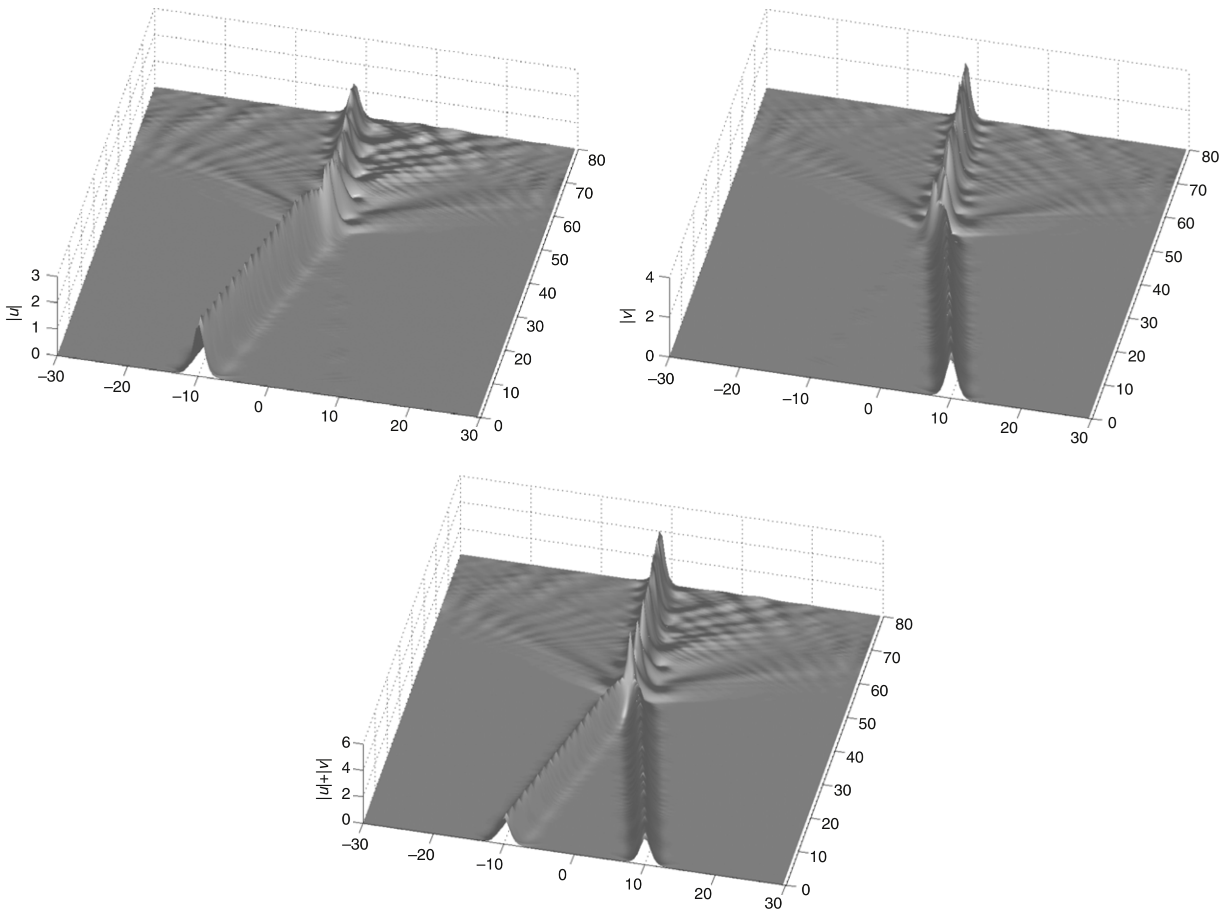

Fig. 5. Fusion of two solitons with $\alpha_1 = 1.0$, $\alpha_2 = -1/3$, $\gamma = 1.0$ and $\Gamma = 0.0175$.

periodic solutions the global energy is preserved more accurately than in case of soliton solutions and global momentum is preserved exactly (up to machine accuracy).

It is well known that the symplectic and multi-symplectic RK methods preserve the linear and quadratic invariants more accurately than the nonlinear ones. Because the global energy in Eq. (19) contains quartic terms, in all soliton solutions the errors in energy preservation are larger than in the global momentum preservation, which contains only quadratic terms.

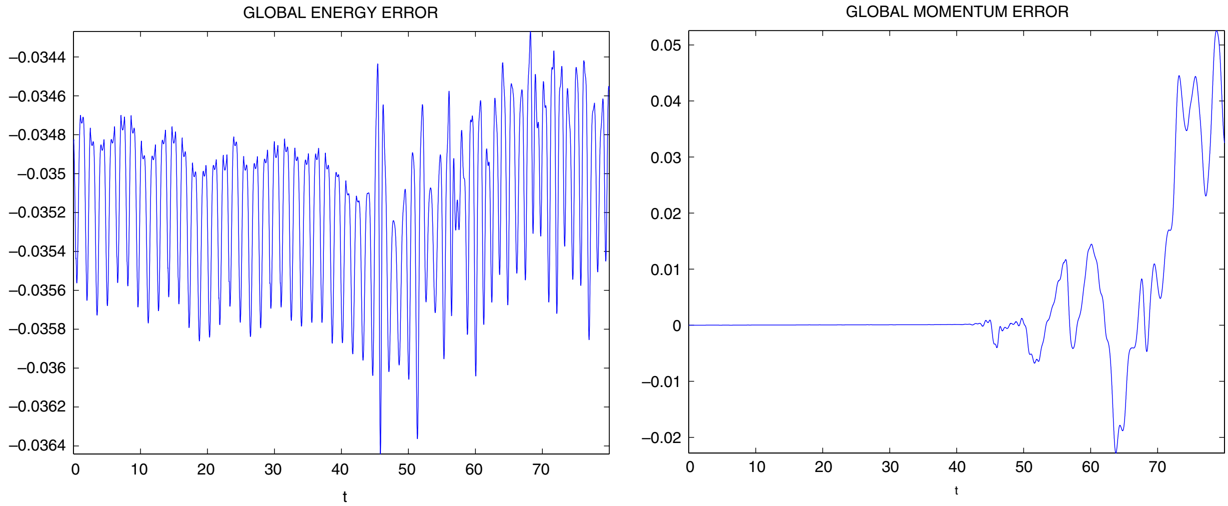

Fig. 6. Global errors for the fusion of two solitons.

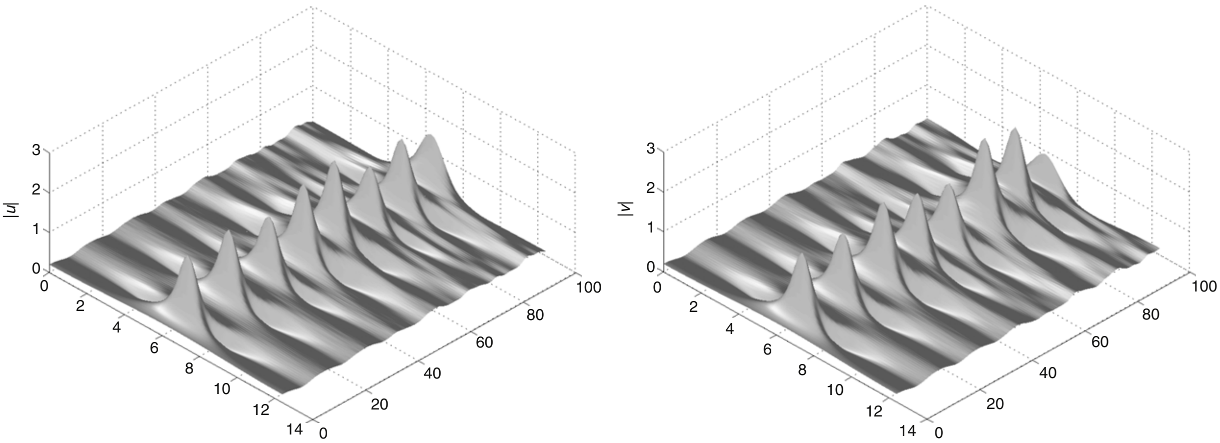

Fig. 7. Periodic solutions with $\alpha_1 = 1.0, \alpha_2 = -1/6, \gamma = 1.0$ and $\Gamma = 0.175$.

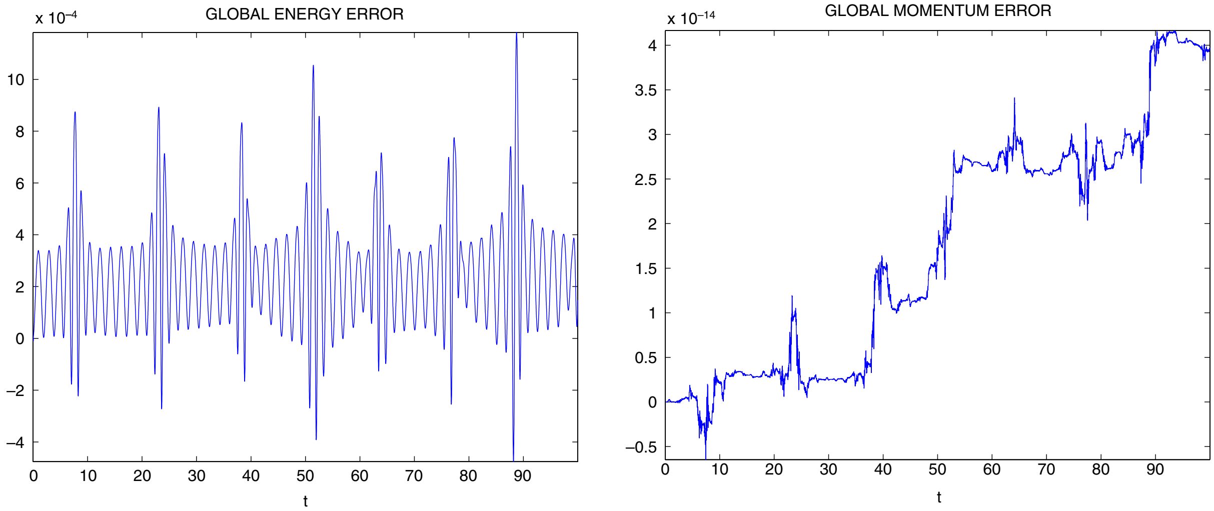

Fig. 8. Global errors for the periodic solutions.

Table 1
Absolute error in mass at various times.

t_n	Elastic collision	Inelastic collision	Fusion of solitons	Periodic solutions
10.0	5.0E−04	5.0E−04	1.0E−04	3.0E−04
20.0	1.0E−04	5.0E−04	4.0E−04	4.0E−04
30.0	9.0E−04	4.0E−04	4.0E−05	3.0E−04
40.0	5.0E−03	9.2E−05	8.0E−04	8.0E−04
50.0	3.8E−03	5.0E−04	5.0E−04	1.9E−04

In Table 1 we give the the absolute errors $Err = |M^0 - M^n|$ for the conservation of the mass (see Eq. (2)) where

$$M^n = \Delta x \sum_{j=1}^{N} ((p_j^n)^2 + (q_j^n)^2 + (\mu_j^n)^2 + (\xi_j^n)^2) \tag{22}$$

is the discrete analog of Eq. (2) at time t_n and M^0 is the initial mass. The exact values of the mass in Eq. (2) for the soliton solutions and the periodic solution are 7.9999 and 6.3146 respectively. Because the mass contains only quadratic terms, it is preserved for all type of solutions.

4. Conclusions

The investigation of solitons arising in non-integrable systems like the SCNLS equation is of great importance both for applications and for understanding the phenomena of soliton propagation. The numerical methods should reflect the dynamical properties of the system and preserve the integral constants like energy, momentum and mass. In this paper semi-explicit multi-symplectic integrator based on Lobatto IIIA–IIIB space and time discretization is developed for the SCLNS equation. The method is more efficient than the implicit conservative and multi-symplectic integrators. It was possible taking non-zero parameter values in the SCNLS equation to study the various solutions including elastic and inelastic collisions, fusion of two solitons and with periodic solutions. The numerical results also showed that global energy, momentum and mass are well preserved in long time integration.

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